

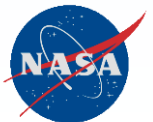
# **Simulations of Turbulent Momentum and Scalar Transport in Confined Swirling Coaxial Jets**

**Tsan-Hsing Shih**

**Ohio Aerospace Institute, Cleveland, OH 44142**

**Nan-Suey Liu and Jeffrey P. Moder**

**NASA Glenn Research Center, Cleveland, OH 44135**



# Objective

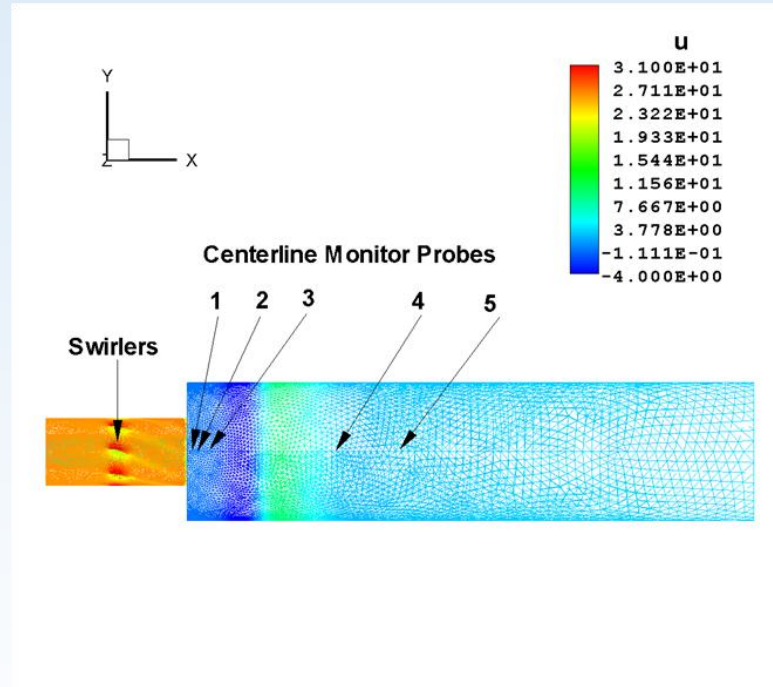
- Validate the newly proposed nonlinear turbulence models for momentum and scalar transport
- Evaluate the newly proposed scalar joint probability density functions (APDF and DWFDf) along with its Eulerian method in the National Combustion Code (NCC).
- Simulations conducted include
  - Steady Reynolds averaged Navier-Stokes RANS,
  - Unsteady RANS (URANS)
  - Time-filtered Navier-Stokes (TFNS) --- very large eddy simulation
  - Hybrid RANS/APDF
  - Hybrid URANS/APDF
  - Hybrid TFNS/DWFDf --- very large eddy simulation

In the hybrid scheme, the transport equations of energy and species are replaced by the APDF or DWFDf equation

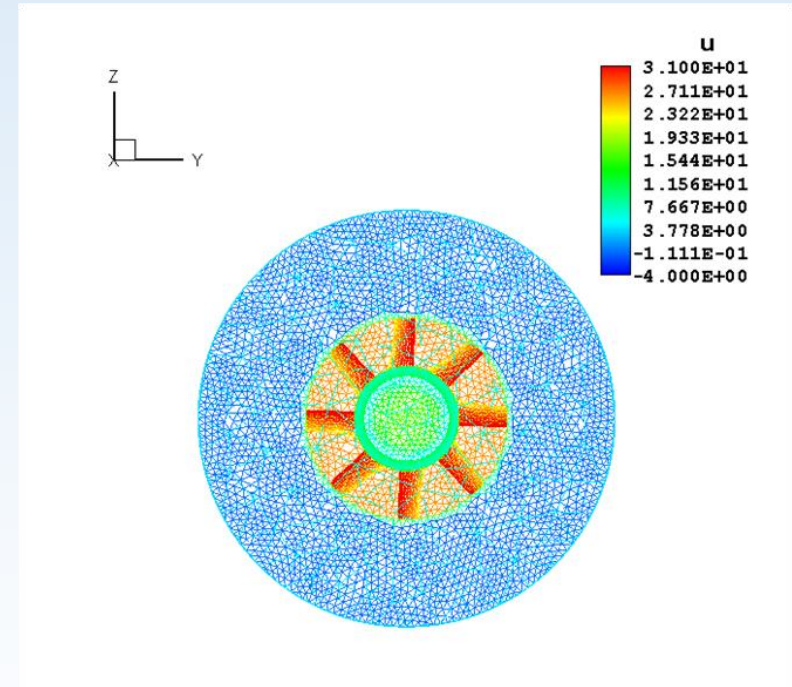
**Some positive effects of nonlinear models and hybrid approaches observed.**

# Confined Swirling Coaxial Jets

## Geometry configuration



## Swirler

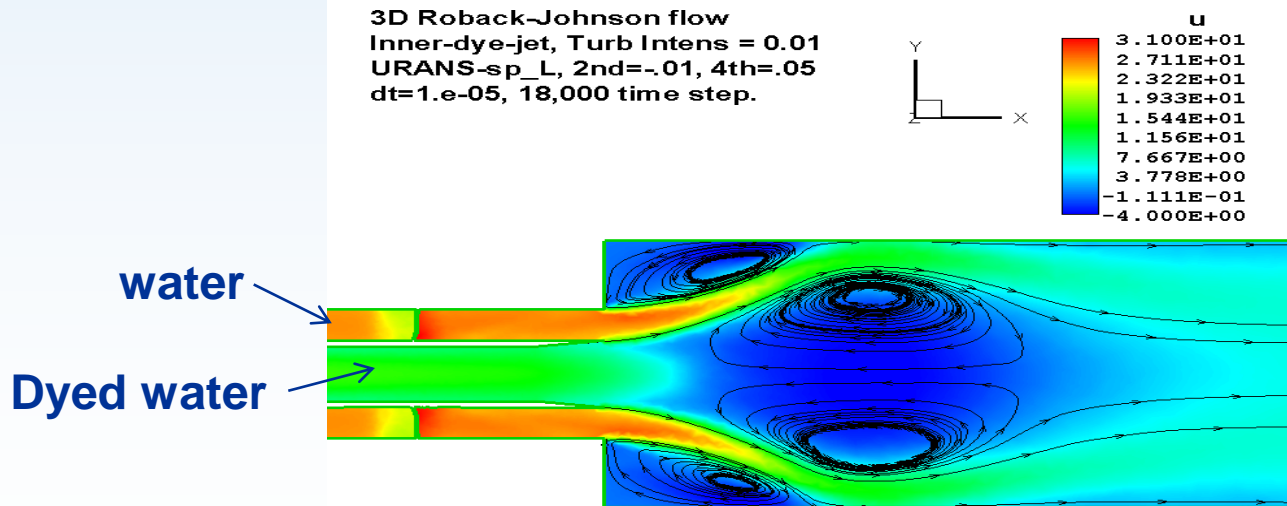


## Computational domain and grid

849,189 tetrahedral elements

# Simulation of water jet using NCC

- Experiments are water jets.
- NCC code is for ideal gas flow.
- “Reynolds number similarity law” under low speed conditions was used for rescaling between the water and gas flows.



# Outline

- **Basic equations for RANS, URANS and TFNS.**
- **Scalar APDF and DWPDF equation for hybrid approach.**
- **Comparison of numerical simulations with experimental data.**
- **Conclusions.**

# Equations for RANS, URANS and TFNS

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} U_j}{\partial x_j} = 0$$

$$\frac{\partial \bar{\rho} U_i}{\partial t} + \frac{\partial \bar{\rho} U_i U_j}{\partial x_j} = -\frac{\partial \bar{P}}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ \nu \left( \frac{\partial \bar{\rho} U_i}{\partial x_j} + \frac{\partial \bar{\rho} U_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial \bar{\rho} U_k}{\partial x_k} \right) \right]$$

$$\frac{\partial \bar{\rho} \tilde{\epsilon}}{\partial t} + \frac{\partial \bar{\rho} U_i \tilde{\epsilon}}{\partial x_i} = -\frac{\partial \bar{q}_i}{\partial x_i} + \overline{PS_{kk}} + \bar{\rho} \tilde{\epsilon} + \bar{Q}$$

$$\frac{\partial \bar{\rho} \Phi_m}{\partial t} + \frac{\partial \bar{\rho} U_i \Phi_m}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \Gamma^{(m)} \frac{\partial \bar{\rho} \Phi_m}{\partial x_i} \right) + \bar{\rho} S_m \quad m = 1, 2, \dots, M$$

$$\bar{P} = \overline{\rho R \sum_{m=1}^M \frac{\Phi_m T}{w_m}} = \overline{\left( \frac{\rho R T}{\bar{M}} \right)} \approx \frac{\bar{\rho} R T}{M} \approx \frac{\bar{\rho} R \Phi_{M+1}}{c_v M}, \quad \frac{1}{\bar{M}} = \sum_{m=1}^M \frac{\Phi_m}{w_m}, \quad \frac{1}{M} = \sum_{m=1}^M \frac{\Phi_m}{w_m}$$

$$\bar{q}_i \approx -\frac{\kappa}{\bar{\rho}} \frac{\partial \bar{\rho} T}{\partial x_i}$$

$$\bar{\phi}(\mathbf{x}, t) = \int_{-\infty}^{+\infty} \phi(\mathbf{x}, t') G(t - t') dt', \quad \phi(\mathbf{x}, t) = \frac{\overline{\rho \phi}}{\bar{\rho}}$$

# Nonlinear models

- $\bar{\rho} U_i U_j, \bar{\rho} U_i e, \bar{\rho} U_i \Phi_m$  can be expressed through the following turbulent transports (stresses and scalar fluxes)  $\tau_{ij}, \Theta_i$  :

$$\tau_{ij} \equiv \bar{\rho} (U_i U_j - \tilde{U}_i \tilde{U}_j), \quad \Theta_i \equiv \bar{\rho} (U_i \theta - \tilde{U}_i \tilde{\theta}).$$

- Nonlinear models are (NASA/TM-1997-113112, 2010-216323):

$$\begin{aligned} \tau_{ij} = & \frac{1}{3} \delta_{ij} \tau_{kk} - 2 C_\mu \cdot f \cdot \bar{\rho} \frac{k^2}{\varepsilon} \left( \tilde{S}_{ij} - \delta_{ij} \tilde{S}_{kk} / 3 \right) - A_3 \cdot f \cdot \bar{\rho} \frac{k^3}{\varepsilon^2} \left( \tilde{S}_{ik} \tilde{\Omega}_{kj} - \tilde{\Omega}_{ik} \tilde{S}_{kj} \right) \\ & + 2 A_5 \cdot f \cdot \bar{\rho} \frac{k^4}{\varepsilon^3} \left[ \tilde{\Omega}_{ik} \tilde{S}_{kj}^2 - \tilde{S}_{ik}^2 \tilde{\Omega}_{kj} + \tilde{\Omega}_{ik} \tilde{S}_{km} \tilde{\Omega}_{mj} - \tilde{\Omega}_{kl} \tilde{S}_{lm} \tilde{\Omega}_{mk} \delta_{ij} / 3 + II_s (\tilde{S}_{ij} - \delta_{ij} \tilde{S}_{kk} / 3) \right], \end{aligned}$$

$$\Theta_i = -\mathcal{G}_T \frac{\partial \bar{\rho} \tilde{\theta}}{\partial x_i} - \mathcal{G}_T \frac{k}{\varepsilon} \left( c_1 \tilde{S}_{ij} + c_2 \tilde{\Omega}_{ij} \right) \frac{\partial \bar{\rho} \tilde{\theta}}{\partial x_j}$$

**where**  $f = 0 \leq f(RCP) \leq 1$ ,  $0 \leq RCP \leq 1$  --- Resolution control parameter.

## Equation for Scalar APDF & DWFDF, $F_{\Phi}(\psi ; \mathbf{x}, t)$

A density weighted ensemble averaged or time filtered fine grained scalar PDF,  $F_{\Phi}(\psi ; \mathbf{x}, t)$ , is defined as:

$$F_{\Phi}(\psi ; \mathbf{x}, t) \equiv \int_{-\infty}^{+\infty} \rho(\mathbf{x}, t') f'_{\Phi}(\psi ; \mathbf{x}, t') G(t - t') dt'$$

where,  $f'_{\Phi}(\psi ; \mathbf{x}, t') \equiv \delta(\Phi(\mathbf{x}, t') - \psi)$  --- fine grained scalar PDF

With above definition, the density weighted mean or filtered variable  $\Phi$  can be fully expressed using  $F_{\Phi}(\psi ; \mathbf{x}, t)$  as:

$$\int_{-\infty}^{+\infty} \psi F_{\Phi}(\psi ; \mathbf{x}, t) d\psi = \overline{\rho \Phi} = \bar{\rho}(\mathbf{x}, t) \Phi(\mathbf{x}, t)$$

Insert this relationship into scalar transport equation, we will obtain a transport equation for scalar  $F_{\Phi}(\psi ; \mathbf{x}, t)$ :



- The resulting transport equation for  $F_\Phi(\psi; \mathbf{x}, t)$  is

$$\frac{\partial F_\Phi}{\partial t} + \frac{\partial (U_i F_\Phi)}{\partial x_i} = \left\{ \frac{\partial}{\partial x_i} \left( \left( \Gamma^{(m)} + \Gamma_T^{(m)} \right) \frac{\partial F_\Phi}{\partial x_i} \right) \right\} - \frac{\partial}{\partial \psi_k} (F_\Phi \cdot S_k(\psi))$$

$$- \frac{\partial}{\partial \psi_k} \left\{ \psi_k \frac{\partial}{\partial x_i} \left( \Gamma_T^{(m)} \frac{k}{\varepsilon} (c_1 S_{ij} + c_2 \Omega_{ij}) \frac{\partial F_\Phi}{\partial x_j} \right) \right\}, \quad k = 1, 2, \dots, M + 1$$

Note that the chemical reaction term  $S_k(\psi)$  is in a closed form!

- The diffusion term in the sample space is further simplified to fit the available PDF solution procedure built in NCC code as

$$- \frac{\partial}{\partial \psi_k} \left\{ \psi_k \frac{\partial}{\partial x_i} \left( \Gamma_T^{(m)} \frac{k}{\varepsilon} (c_1 \tilde{S}_{ij} + c_2 \Omega_{ij}) \frac{\partial F_\Phi}{\partial x_j} \right) \right\} \approx \frac{\partial}{\partial \psi_k} \left( \psi_k \frac{1}{\tau} F_\Phi \right)$$

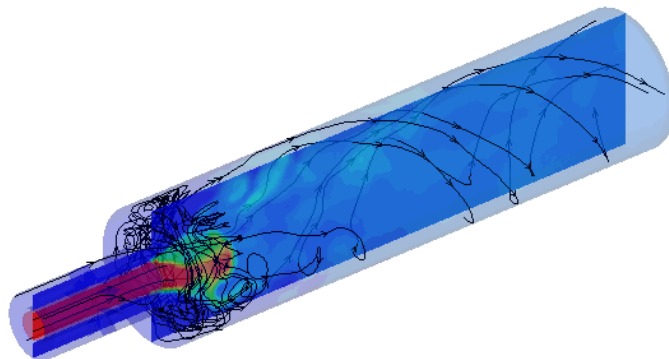
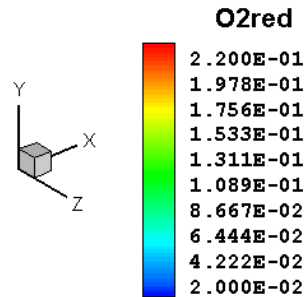
$$\text{where, } \frac{1}{\tau} \equiv \sqrt{\tilde{S}_{ij} \tilde{S}_{ij} + \Omega_{ij} \Omega_{ij}}$$

# Results of simulations and comparisons

# Global flow features of TFNS (VLES) simulation

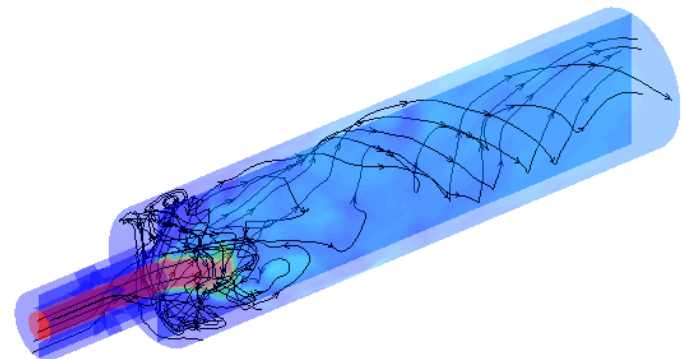
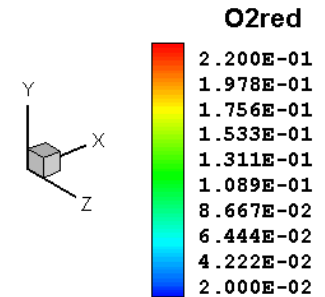
## Scalar flux model: linear

3D Roback-Johnson flow  
Inner-dye-jet, Turb Intens = 0.01  
TFNS with sp\_L, wf, 2nd=0, 4th=.05  
dt=2.e-06, 335,000 time step.



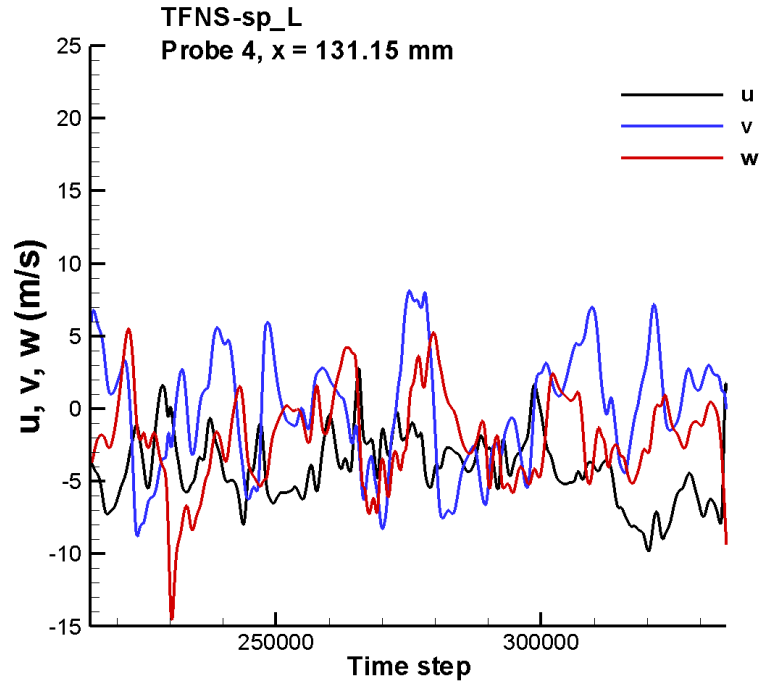
## Scalar flux model: non-linear

3D Roback-Johnson flow  
Inner-dye-jet, Turb Intens = 0.01  
TFNS with sp\_nl, wf, 2nd=0, 4th=.05  
dt=2.e-06, 335,000 time step.

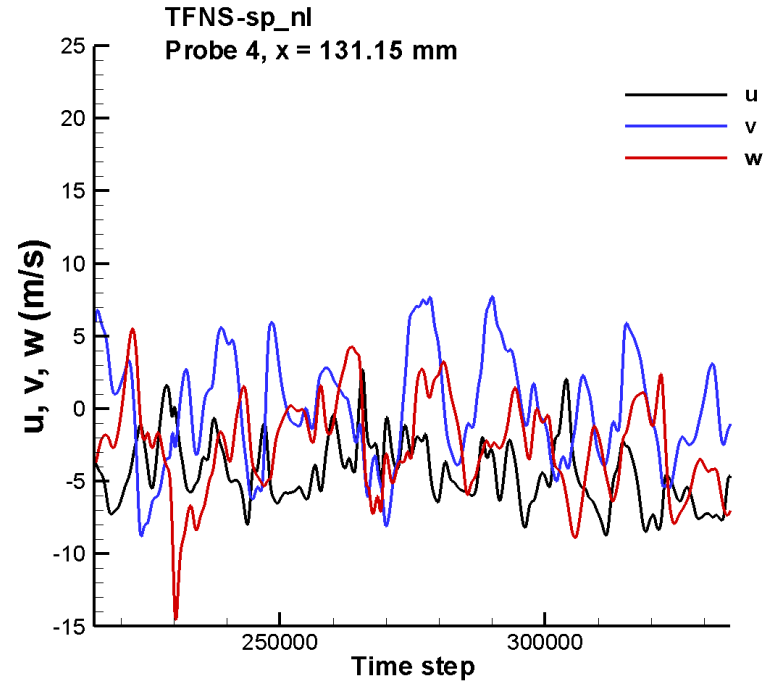


# Time history of velocity components $u$ , $v$ , $w$ at probe 4

## Scalar flux model: linear



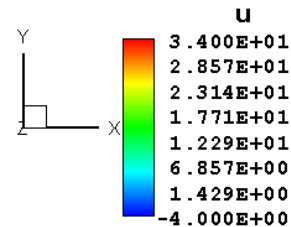
## Scalar flux model: non-linear



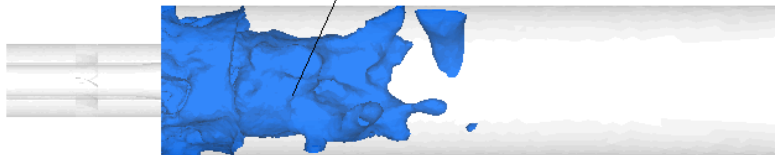
# Vortex brake-down Bubble

## Scalar flux model: linear

3D Roback-Johnson flow  
Inner-dye-jet, Turb Intens = 0.01  
TFNS with sp\_L, wf, 2nd=0, 4th=.05  
dt=2.e-06, at 335,000 time step

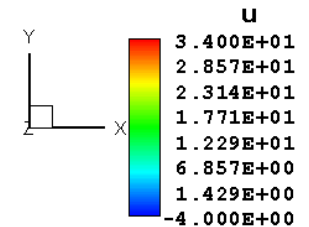


Iso-surface of  $U=0$

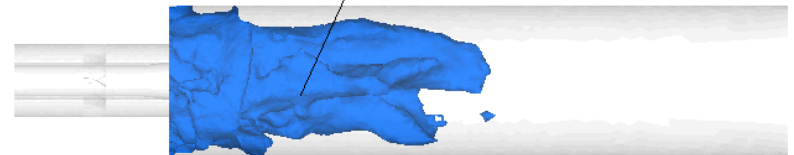


## Scalar flux model: non-linear

3D Roback-Johnson flow  
Inner-dye-jet, Turb Intens = 0.01  
TFNS with sp\_nl, wf, 2nd=0, 4th=.05  
dt=2.e-06, at 335,000 time step



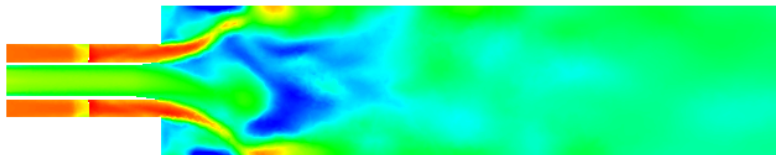
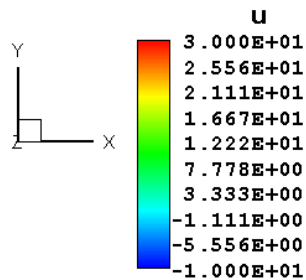
Iso-surface of  $U=0$



# Contour of instant axial velocity, $u$

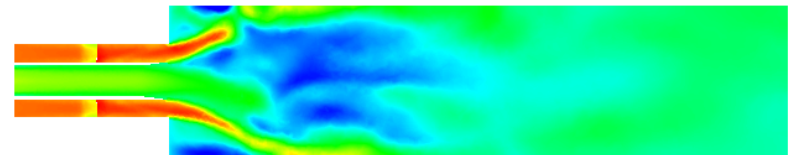
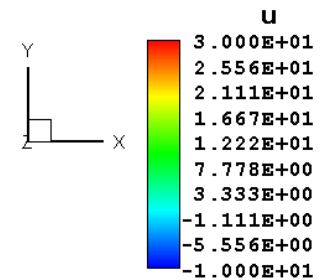
## Scalar flux model: linear

3D Roback-Johnson flow  
Inner-dye-jet, Turb Intens = 0.01  
TFNS with sp\_L, wf, 2nd=0, 4th=.05  
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## Scalar flux model: non-linear

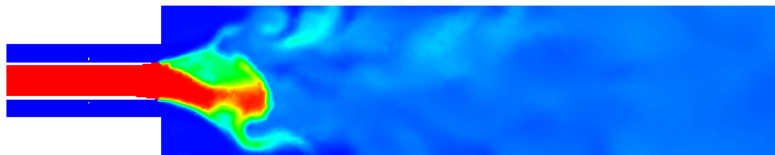
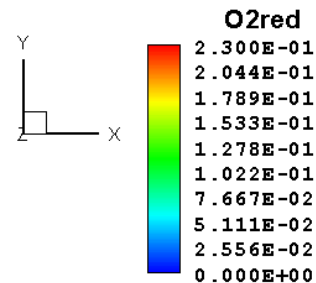
3D Roback-Johnson flow  
Inner-dye-jet, Turb Intens = 0.01  
TFNS with sp\_nl, wf, 2nd=0, 4th=.05  
dt=2.e-06, at 335,000 time step



# Contour of colored O2 concentration

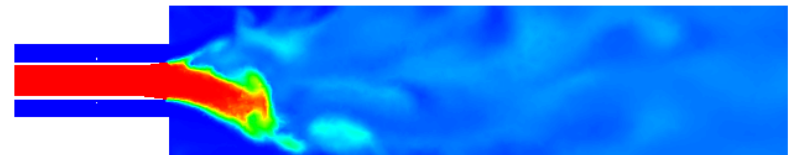
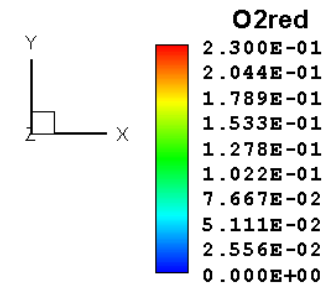
## Scalar flux model: linear

3D Roback-Johnson flow  
Inner-dye-jet, Turb Intens = 0.01  
TFNS with sp\_L, wf, 2nd=0, 4th=.05  
dt=2.e-06, at 335,000 time step



## Scalar flux model: non-linear

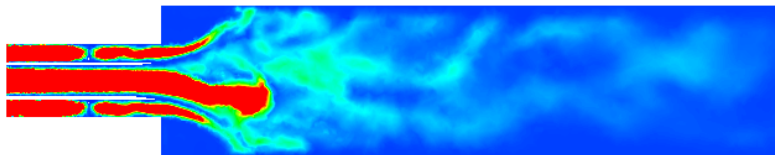
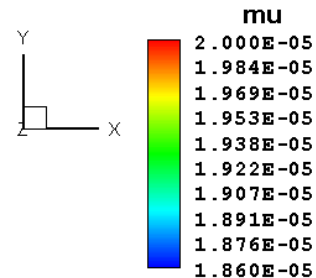
3D Roback-Johnson flow  
Inner-dye-jet, Turb Intens = 0.01  
TFNS with sp\_nl, wf, 2nd=0, 4th=.05  
dt=2.e-06, at 335,000 time step



# Contour of effective viscosity, $\mu$

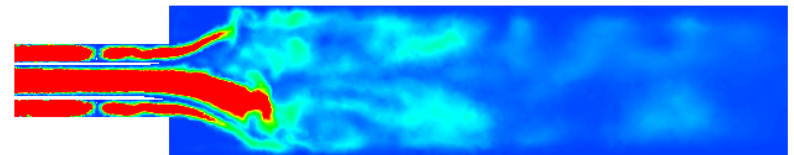
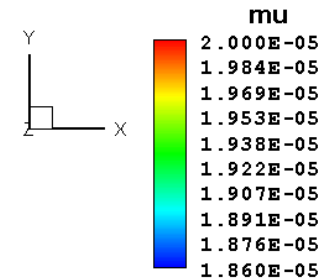
## Scalar flux model: linear

3D Roback-Johnson flow  
Inner-dye-jet, Turb Intens = 0.01  
TFNS with sp\_L, wf, 2nd=0, 4th=.05  
dt=2.e-06, at 335,000 time step



## Scalar flux model: non-linear

3D Roback-Johnson flow  
Inner-dye-jet, Turb Intens = 0.01  
TFNS with sp\_nl, wf, 2nd=0, 4th=.05  
dt=2.e-06, at 335,000 time step

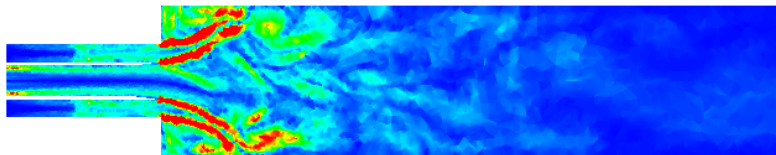
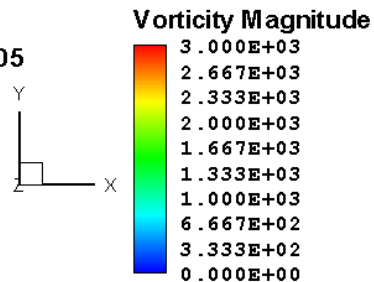




# Contour of vorticity magnitude

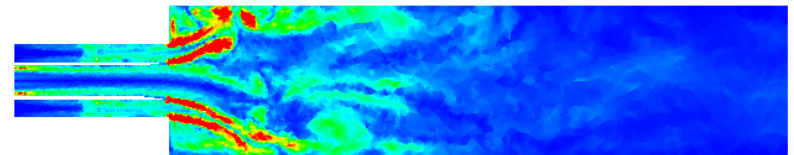
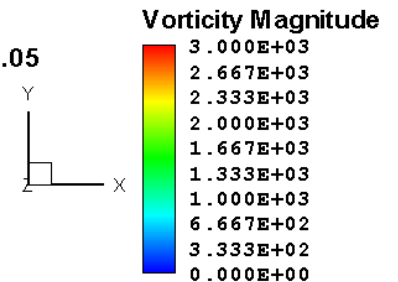
## Scalar flux model: linear

3D Roback-Johnson flow  
Inner-dye-jet, Turb Intens = 0.01  
TFNS with sp\_L, wf, 2nd=0, 4th=.05  
dt=2.e-06, at 335,000 time step

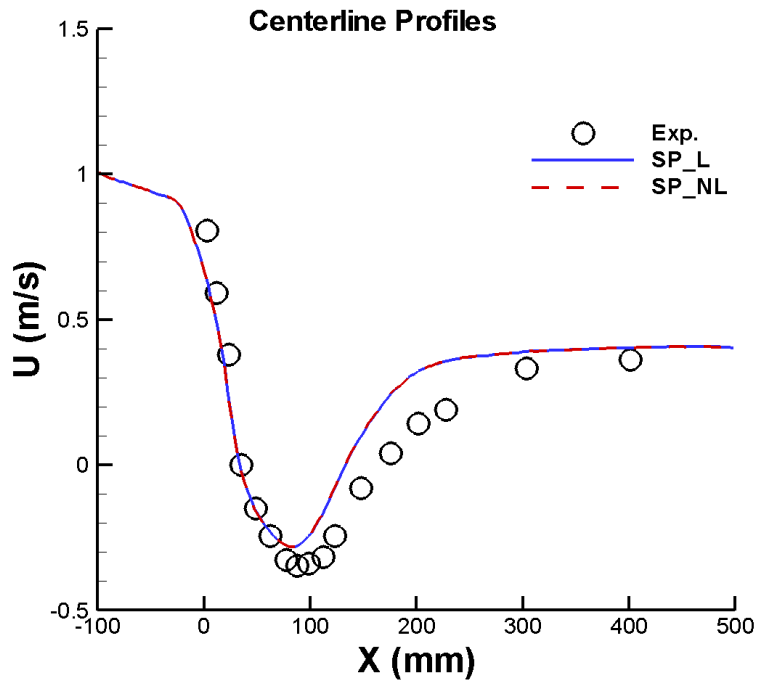


## Scalar flux model: non-linear

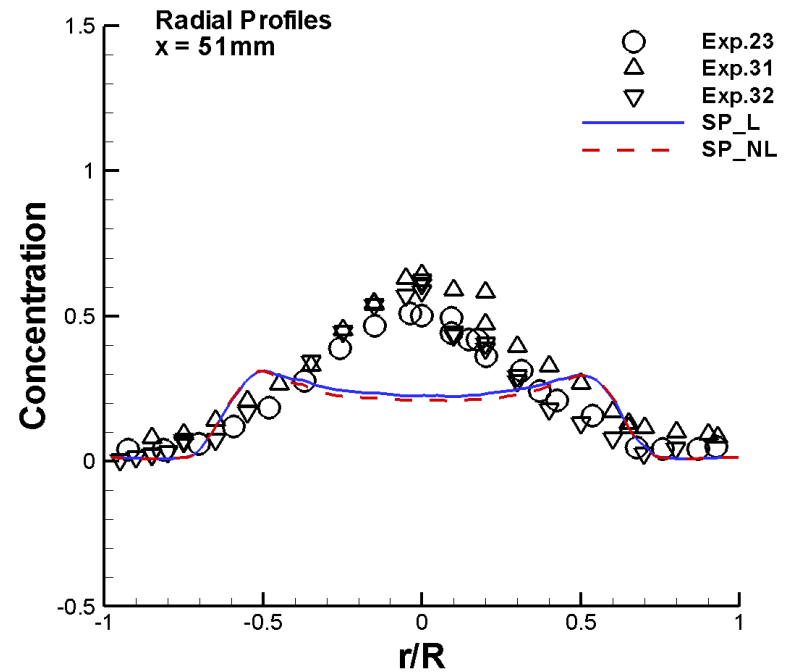
3D Roback-Johnson flow  
Inner-dye-jet, Turb Intens = 0.01  
TFNS with sp\_nl, wf, 2nd=0, 4th=.05  
dt=2.e-06, at 335,000 time step



# URANS simulation

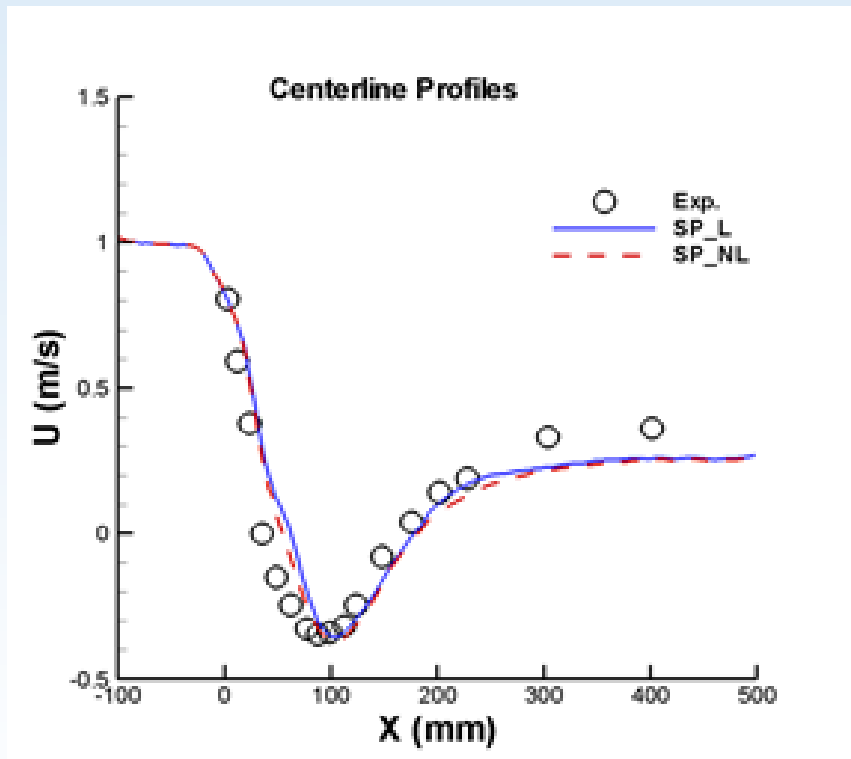


URANS: Axial velocity along centerline

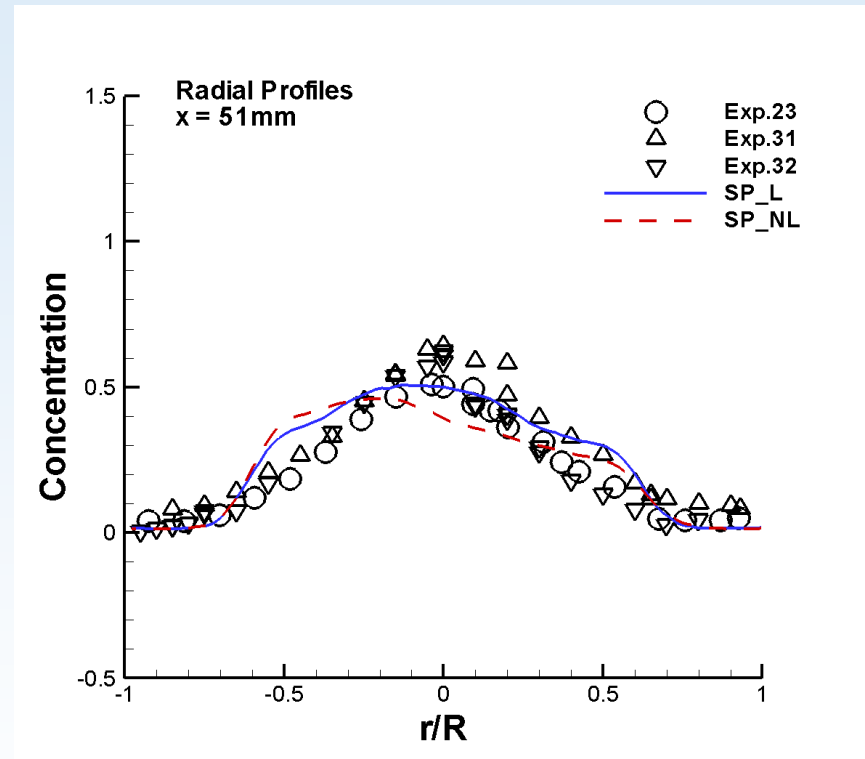


Inner Jet concentration at downstream

# TFNS (VLES) simulation

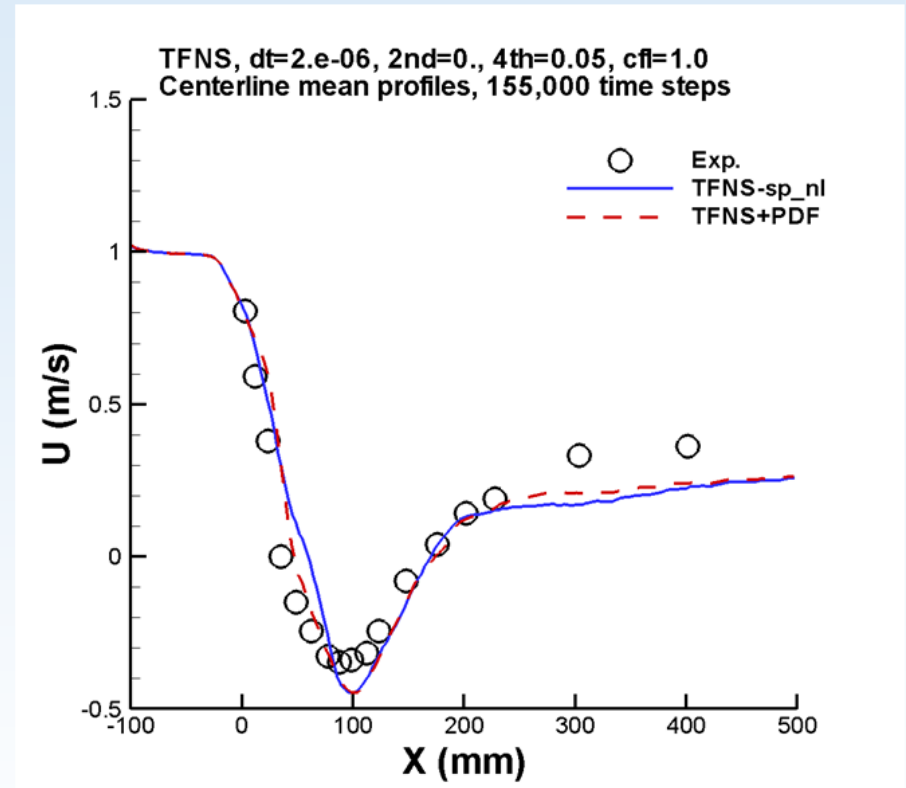
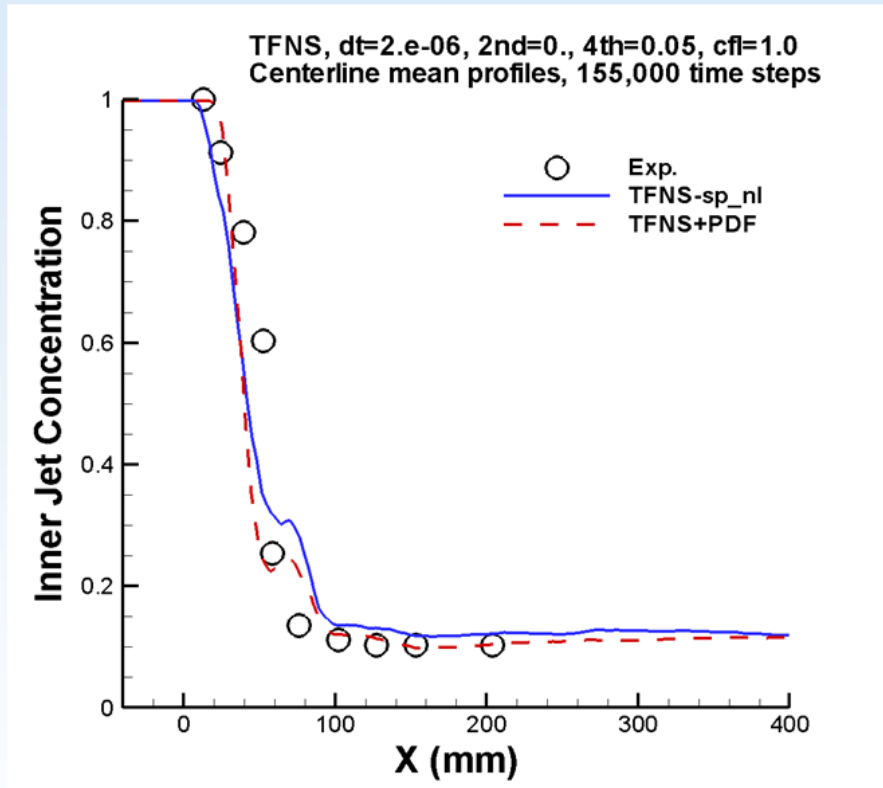


TFNS: Axial velocity along centerline



Inner Jet concentration at downstream

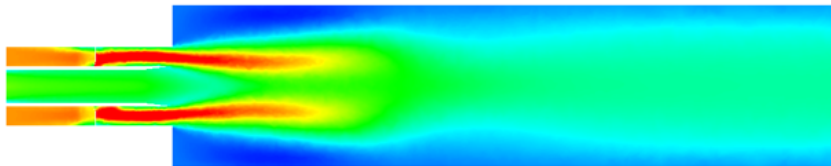
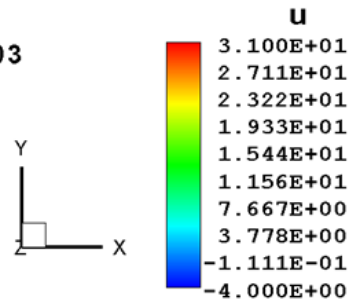
# Hybrid TFNS/DWFDF vs. TFNS



Mean concentration and axial velocity distribution along the centerline  
Positive improvements shown from hybrid method

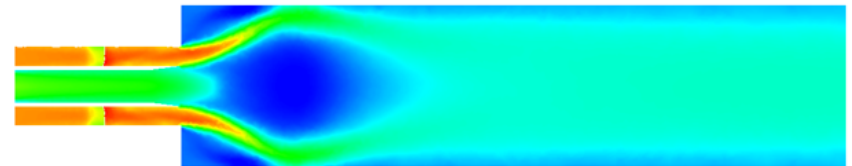
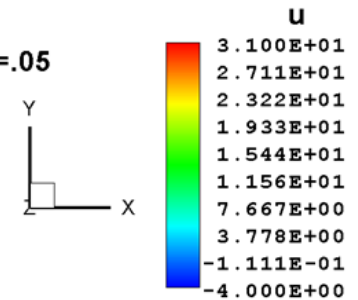
# Appendix: RANS simulation standard $k - \varepsilon$ model vs. nonlinear model

RANS standard k-eps model with WF  
cfl=1.0, 2nd=-.01, 4th=.05, conv=1.e-03  
converged at 155,224 iteration



Center recirculation zone missed

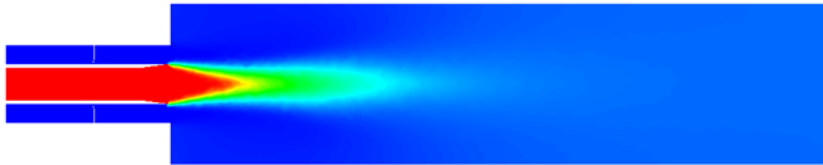
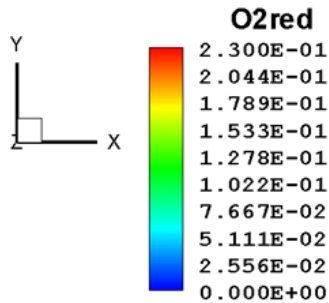
3D Roback-Johnson flow  
Inner-dye-jet, Turb Intens = 0.01  
RANS-NL-wf, cfl=1.0, 2nd=-.01, 4th=.05  
At 153,224 iteration, converged



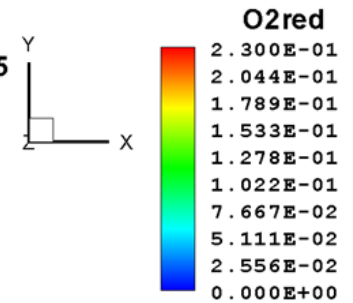
Center recirculation zone

# Appendix: RANS simulation standard $k - \varepsilon$ model vs. nonlinear model

RANS standard k-eps model with WF  
cfl=1.0, 2nd=-.01, 4th=.05, conv=1.e-03  
converged at 155,224 iteration

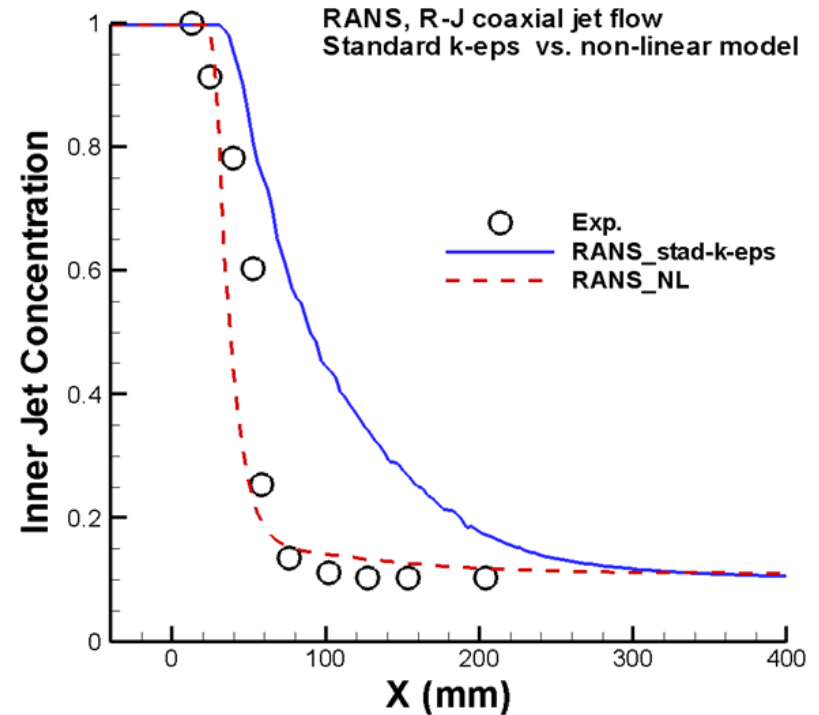
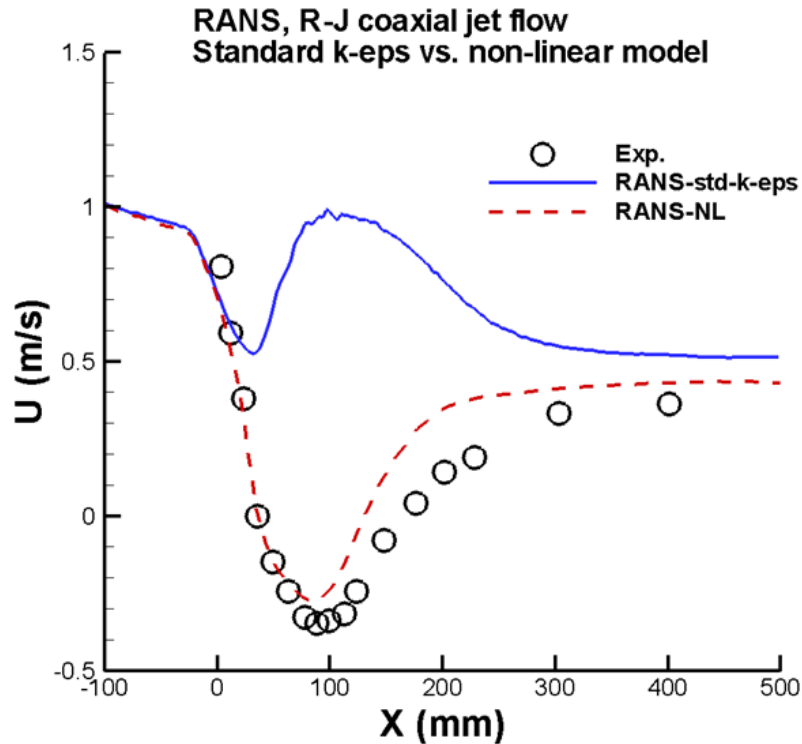


3D Roback-Johnson flow  
Inner-dye-jet, Turb Intens = 0.01  
RANS-NL-wf, cfl=1.0, 2nd=-.01, 4th=.05  
At 153,224 iteration, converged



Contour of inner jet concentration at center plane (x,y)

# Appendix: RANS simulation standard $k - \varepsilon$ model vs. nonlinear model



Axial velocity and concentration along the centerline

# Conclusions

- Two groups of validations have been performed against experimental data:
  - The first group focuses on the turbulent scalar flux models: linear vs. nonlinear. Simulations include RANS, URANS and TFNS.
  - The second group focuses on the hybrid approach. Simulations include RANS/APDF, URANS/APDF and TFNS/DWFDF.
- Regarding the scalar flux model:
  - the linear and nonlinear scalar flux models have the same or similar behavior in RANS, URANS and TFNS simulations.
  - In the case of TFNS simulation, TFNS results demonstrate significant improvements over their RANS and URANS counterparts.
- Regarding the hybrid approach:
  - RANS/APDF, URANS/APDF and TFNS/DWFDF simulations show that they are quite close to their respective RANS, URANS and TFNS counterparts.
  - The hybrid approach appears to be more robust in the unsteady calculations and converge faster to use less computing time.
  - The above observations show a quite positive opinion of present hybrid PDF method for even non-reacting flow simulations.